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INTERIM SCIENTIFIC REPORT

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November 1, 1983 - October 31, 1984

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INTRODUCTION

Our work during this period continued to have as its main objective the study of (a) the thermodynamics and structure of plasmas and dense molecular fluids and (b) the distribution of the microfield in a strongly coupled plasma. Our research included both rigorous analysis and approximation schemes.

We continued applying our medium approximation to a variety of systems. This method continues to be the simplest scheme available for dealing with dense diatomic fluids. It also seems to work reasonably well for simple mixtures. In fact, we found a new scheme for reducing a mixture to a one component fluid, which we hope to explore further.

In the area of plasmas our APEX approximation seems to be the best one around for static microfield distribution. We have, during the last year, obtained some new results about the time dependent gas, but no simple approximation scheme yet.

Our work has been in close collaboration with groups at Los Alamos National Laboratory and at Lawrence Livermore National Laboratory. We give here a brief description of the work and attach publications.

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1. On Potential and Field Fluctuations in Classical Charged Systems

(J. L. Lebowitz and Ph. A. Martin)

Using electrostatic identities the potential and microfield in a plasma, important for determining line shapes, are expressed as limits of local quantities. These are shown to be well defined for typical configurations of macroscopic, i.e. infinite systems (under some mild clustering assumptions). Their covariance contains a slowly decaying part ($|x|^{-1}$, for the potential) whose coefficient is universal whenever the Stillinger-Lovett second moment condition holds. We show further that the contributions from distant regions (which are equal to suitable averages over local regions) have a Gaussian distribution.

(Appeared in Jour. Stat. Phys., Vol. 34, Nos. 1/2, 1984) Reprints under separate cover

2. Low-Frequency Component Electric Microfield Distributions in Plasmas

(Carlos A. Iglesias, Joel L. Lebowitz, David MacGowan and Hugh E. DeWitt)

We evaluate the low-frequency component electric microfield distribution at a charged point, i.e. the field distribution in a gas of ions interacting through a Yukawa potential. The method employed is an adaptation of the APEX approximation previously developed for the high-frequency component and involves a noninteracting quasi-particle representation of the screened plasma designed to yield the correct second moment of the microfield distribution. The APEX results are compared to new Monte Carlo simulations at various plasma coupling strengths and we find good agreement. In connection with this analysis we also solved the hypernetted chain approximation for the Yukawa potential and compared that to the Monte Carlo simulations.

(To appear in Phys. Rev. A, tent. pub. date March 1985) Reprints under separate cover when available

3. Thermodynamics of Homonuclear Diatomic Fluids from the Angular Median Potential

(David MacGowan, Eduardo M. Waisman, Jool L. Lobowitz and Jerome K. Percus)

The use of the angular median potential as a temperature-independent spherical reference system for approximating molecular fluids is tested for its predictions of thermodynamics. Calculations have been carried out for a wide range of homonuclear diatomics with continuous atom-atom potentials believed to be representative of the full range of simulation data available for such systems. The results for the pressure are surprisingly good both in the detonation regime and around the triple point. In the latter case, however, the internal energies for highly elongated molecules with attractive potential wells are considerably too positive. Comparison with other perturbation theories indicates that the median reference system gives better pressures but poorer energies than RAM, and that in many cases, especially for purely repulsive potentials, it gives results of comparable accuracy to those obtained with non-spherical reference systems.

(Appeared in J. Chem. Phys. 80(6), 15 March 1984) Reprints under separate cover

4. Spherical Reference Systems for Non-Spherical Hard Interactions

(G. O. Williams, J. L. Lebowitz and J. K. Percus)

We investigate the applicability of the median and Barker-Henderson prescriptions for obtaining spherical reference systems for three models: hard linear triatomics, hard heteronuclear dumbbells, and two-component mixtures of hard dumbbells. We propose an empirical method for determining the median potential for

systems lacking a high degree of symmetry. For mixtures of hard molecules, we find that both the median and Barker-Henderson prescriptions give rise to approximately additive hard sphere reference potentials.

(Appeared in J. Phys. Chem., December 1984) Reprints under separate cover when available

5. Monte Carlo Simulation of Hard Spheroids

(J. W. Perram, M. S. Wertheim, J. L. Lebowitz and G. O. Williams)

We present Monte Carlo simulations of the equation of state and radial distribution function for a model fluid composed of hard spheroids.

(Appeared in Chem. Phys. Letts., Vol. 105, No. 3, 16 March 1984)
Reprints under separate cover

6. Electric Microfield Distributions in Multicomponent Plasmas

(Carlos A. Iglesias and Joel L. Lebowitz)

We evaluate the electric microfield distribution in a multicomponent plasma (MCP). The method employed is an adaption of the very simple adjustable-parameter exponential approximation previously developed for one-component plasmas (OCP). We also discuss a still simpler approximation in which the MCP is replaced by an effective OCP. The results are generally close to each other and the former is in very good agreement with computer simulations.

(Appeared in Phys. Rev. A, Vol. 30, No. 4, October 1984) Reprints under separate cover

7. One Molecular Fluid Approximation for Diatomic Fluid Mixtures
(Eduardo M. Waisman, Joel L. Lebowitz and David MacGowan)

We investigate a one component molecular fluid approximation for conformally similar molecules. We test this scheme on (two) mixtures of rigid homonuclear diatomic Lennard-Jones (LJ) fluids for which a limited amount of information from molecular dynamics simulations is available. For two components of approximately equal bond length but different LJ parameters our results compare favorably with the machine computations. From the very few simulation data available for equimolar mixtures of molecules differing only in their bond lengths we cannot reach any firm conclusion. Alternative procedures for treating general molecular fluid mixtures are discussed.

(Appeared in Jour. Chem. Phys., 15 December 1984) Reprints under separate cover when available

8. New Systematic Expansion of the Electric Field Distribution in Plasmas

(Angel Alastuey, Carlos A. Iglesias, Joel L. Lebowitz and Dominique Levesque)

We derive a new systematic expansion of the electric field distribution at a test charge immersed in an infinite two- or three-dimensional one-component plasma. The lowest order truncation of this expansion leads to a mean field theory very similar to the Adjustable Parameter Exponential Approximation (APEX). The next order corrections to this mean field theory are explicitly computed in terms of the distribution functions of the plasma particles. All these approximations are compared to the Monte Carlo results for a two-dimensional system at $\Gamma = 2$ and various test charges. The systematic approximations appear to be useful. Even the zeroth-order approximation is quite accurate for large test charges or strongly coupled systems and the next order improves on it. Still APEX is found to be most reliable (as it is also in three dimensions) and remains accurate in the practically interesting limit where the test charge vanishes, i.e. at a neutral atom.

(Appeared in Phys. Rev. A, Vol. 30, No. 5, November 1984) Reprints under separate cover

9. The Two-Dimensional One-Component Plasma in an Inhomogeneous Background: Exact Results

(A. Alastuey and J. L. Lebowitz)

We study the general inhomogeneous two-dimensional jellium where the background density varies in one space direction only. At $r = 2$, explicit functional representations of the one- and two-body densities of the particles are derived in terms of the electrostatic potential created by the background. The present model can be used for describing a large variety of charged interfaces.

(Appeared in J. Physique 45, pp. 1859-1874, December 1984) Reprints under separate cover

10. Van der Waals One-Fluid Theory: Justification and Generalisation

(David MacGowan, Joel L. Lebowitz and Eduardo M. Waisman)

We describe an approach to Van der Waals one-fluid theory based on thermodynamic consistency and propose a method for generalising it to non-conformal fluids.

(To appear in Chem. Phys. Letts.) Preprint under separate cover

11. Long Wave Length Oscillations in an Inhomogeneous One Component Plasma

(Joel L. Lebowitz and Ph. A. Martin)

The perfect screening of charge fluctuations in an equilibrium plasma is extended to the time displaced structure function of a general inhomogeneous one component plasma. We find that the long wavelength modes oscillate undamped with a single frequency $\bar{\omega}$, $\bar{\omega}^2$ being an angular average of squares of plasma frequencies $\omega_p^2 = \frac{4\pi e^2 \rho}{m}$ in uniform systems with density ρ . Our results are derived rigorously from the BBGKY hierarchy under some reasonable assumptions on the spatial decay of correlations and contains as special cases previously obtained results of this kind.

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12. Angular Correlations in Dense Hot Diatomic Fluids

(David MacGowan, James Daniel Johnson and Milton Samuel Shaw)

Molecular dynamics (MD) simulation data for rigid diatomic models of N_2 and CO_2 under conditions of extremely high density and temperature are analyzed for static correlation functions. The results show some significant qualitative differences from those for diatomic fluids at normal densities and temperatures (i.e., near the triple point). For a single thermodynamic state of N_2 , the radial distribution functions (RDFs) of the (spherical) RAM and median potentials are found, also by MD. Whereas the median gives good thermodynamic results and poor centers correlation functions, RAM produces just the opposite. Thus no explanation in terms of distribution functions is found for the success of the median for thermodynamics although an empirical correlation is found between the breakdown of median thermodynamics for CO_2 and a distinctive feature of the molecular correlation functions.

(To appear in Jour. Chem. Phys.) Reprints under separate cover when available

13. Exact Results for the Two-Dimensional One-Component Plasma

(D. Nicolaides)

We show that the free energy and correlation functions of the 2D OCP at the special temperature $T_0 = e^2/2k_B$ can be explicitly computed by solving a free-field Dirac equation.

(Appeared in Phys. Letts., Vol. 103A, No. 5, 9 July 1984) Reprints under separate cover

14. Exact Results for the Two-Dimensional Two-Component Plasma

(D. Nicolaides)

The free energy and correlation functions of a two-dimensional two-component Plasma are explicitly computed at the special temperature $T_0 = e^2/2k_B$.

(Appeared in Phys. Letts., Vol. 103A, No. 1,2, 18 June 1984) Reprints under separate cover

15. Equivalent Potentials for Equations of State for Fluids of Non-spherical Molecules

(G. O. Williams, J. L. Lebowitz and J. K. Percus)

We analyze the extent to which the equation of state and other thermodynamic properties of systems of hard nonspherical molecules can be obtained from a density independent hard sphere reference system. We conclude that the median and Barker-Henderson prescriptions effectively reproduce all data now available. We discuss the motivation for these two formulations in detail.

(Appeared in J. Chem. Phys., 81(4), 15 August 1984) Reprints under separate cover

16. The Ideally Polarizable Interface: Integral Equations

(M. L. Rosinberg, L. Blum and J. L. Lebowitz)

The integral equations used in the microscopic theory of the electric double layer are extended to the case of an impermeable interface separating two conducting media. (ionic solutions, or plasmas). This system is a model for an ideally polarizable interface. Exact relations are given for the contact values of the one particle density function, and also for the pair correlation functions.

We solve numerically the Poisson-Boltzmann (PB), the Hypernetted Chain (HNC) and Mean Spherical (MSA) approximations, and compare the results to the exact solution of the one component plasma in two dimensions.

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PUBLICATIONS WHICH HAVE APPEARED SINCE
1982-1983 INTERIM SCIENTIFIC REPORT

1. On Potential and Field Fluctuations in Classical Charged Systems. Jour. Stat. Phys., 34, 1/2, pp. 287-311, 1984
(J. L. Lebowitz and Ph. A. Martin) Reprints under separate cover
2. Thermodynamics of Homonuclear Diatomic Fluids from the Angular Median Potential. J. Chem. Phys. 80(6), 15 March 1984
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8. Exact Results for the Two-Dimensional One-Component Plasma. Phys. Letts., 103A, 5, 9 July 1984
(D. Nicolaides) Reprints under separate cover
9. Effective Spherical Potentials for the Thermodynamics of Homonuclear Diatomic Lennard-Jones Liquids. Jour. Chem. Phys., 81(7), 1 October 1984
(David MacGowan)
10. The Self-Consistent Mean Spherical Approximation for the One-Component Plasma. Jour. Stat. Phys., 32, 1, 1983
(David MacGowan)
11. Fluids with Highly Directional Attractive Forces. I. Statistical Thermodynamics. Jour. Stat. Phys., 35, 1/2, 1984
(M.S. Wertheim)
12. Fluids with Highly Directional Attractive Forces. II. Thermodynamic Perturbation Theory and Integral Equations. Jour. Stat. Phys., 35, 1/2, 1984
(M. S. Wertheim)

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